2-(Hydroxymethyl)-2-methyl-1,3-propanediol
77-85-0 | DTXSID2026444

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 171 °C

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
2-(Hydroxymethyl)-2-methyl-1,3-propanediol	Glycerol	1,3-Propanediol, 2-(bromomethyl)-2-(hydroxymethyl)-
Measured: 204	**Measured:** 18.2	**Measured:** 76.0
Predicted: 171	**Predicted:** 52.1	**Predicted:** 94.7